

Supplementary TABLE 1: NMR (500MHz) in CDCl₃

A. Oc-3 (GGL)				B. Oc-3 (GGL) triacetate			
Carbon no	¹ H	¹³ C	HMBC	Carbon no	¹ H	¹³ C	HMBC
1	4.2-4.3(2H)	62.6(62.7)	3	1	4.1, 4.3(2H)	62.7	3
2	5.26	70.5	1, 3	2	5.19	70.1	1, 3
3	3.6-3.7, 3.98	68.7	1'	3	3.66, 3.96	68.1	1'
1'	4.22	104.0	2', 3	1'	4.47	102.0	2', 3
2'	3.61-3.62	72.0 or 73.5	4', 3'	2'	5.18	69.1	*(2.06, CH ₃ -COO-) 1', 3'
3'	3.61-3.62	73.5 or 72.0	4', 2'	3'	5.01	71.2	*(1.98, CH ₃ -COO-) 2', 4'
4'	3.89	68.4	5', 6'	4'	5.36	67.3	*(2.06, CH ₃ -COO-) 5', 6'
5'	3.67	72.8	6'	5'	3.9	71.2	4', 6'
6'	4.2-4.3, 4.39	62.7(62.6)	5'	6'	4.1-4.2	61.3	5'
1"	-	173.8 173.9, 174.3	2, 2" 1, 6"	1"	-	173.7 173.2 170.6 169.8	2', 3', 6" 2', 3', 6" *(1.98, 2.15 CH ₃ -COO-) 2" *(2.06 CH ₃ -COO-) 2"
2"	2.32	34.5, 34.7	3", 4"	2"	2.30	34.3- 34.6	3"
3"	1.61	25.3	2", 4"	3"	1.59	25.1, 25.3	2", 4"
4"-7"	1.25-1.30	29.5-30.1	2", 3", 8", 9"	4"-7"	1.25-1.30	29.5-30.0	2", 3"
8"	2.06	27.6	7", 9", 10"	8"	2.06	27.6	9", 10", 16"
9"	5.3-5.4	128.2, 130.6	8", 11"	9"	5.3-5.4	128.2, 130.6	8", 11"
10"	5.3-5.4	128.2, 130.6	8", 11"	10"	5.3-5.4	128.2, 130.6	8", 11"
11"	2.8	25.9, 26.0	9", 10", 12", 13", 15", 16"	11"	2.8	25.9, 26.0	9", 10", 12", 13", 15", 16"
12"	5.3-5.4	128.6, 128.7	11", 14"	12"	5.3-5.4	128.6, 128.7	11", 14"
13"	5.3-5.4	128.6, 128.7	11", 14"	13"	5.3-5.4	128.6, 128.7	11", 14"
14"	2.8	25.9, 26.0	12", 13", 15", 16"	14"	2.8	25.9, 26.0	9", 10", 12", 13", 15", 16"
15"	5.3-5.4	127.5	14", 17"	15"	5.3-5.4	127.5	14", 17"
16"	5.3-5.4	132.4	14", 17", 18"	16"	5.3-5.4	132.4	14", 17", 18"
17"	2.07	20.9	15", 16", 18"	17"	2.06	~ 20.9 overlap by acetate signal	15", 16", 18"
18"	0.98	14.7	16", 17"	18"	0.98	14.7	16", 17"

* Assignments are tentative due to overlap

Supplementary TABLE-1. Detailed NMR assignments of Oc-3 and its acetate which was derived from 2D NMR spectrometric analysis (¹H-¹H COSY, NOESY, ¹H-¹³C HMQC, ¹H-¹³C HMBC)

